HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

Low Benzene Naphtha Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

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PLAIN ENGLISH SUMMARY

This category test plan addresses nine petrochemical streams (products) derived from the ethylene and associated manufacturing processes. The category has been designated "Low Benzene Naphtha." The category includes complex products that are mixtures containing primarily C5 through C12 olefins, paraffins, naphthenes, and aromatic molecules. The benzene content of these streams is typically less than two percent but in some cases may be as high as five percent. The Low Benzene Naphtha Category streams share many of the same components as the gasoline blending streams referenced in the American Petroleum Institute Petroleum HPV Testing Group Gasoline Blending Streams Test Plan. In fact, some of the Low Benzene Naphtha Category streams are used as gasoline blending stock. Based upon existing information plus data and information that will be developed as outlined in this test plan, a scientifically based characterization of the HPV Program endpoints for this category will be possible.

Human Health Effects

The strategy for characterizing human health hazards of products in this category is to evaluate data on similar complex mixtures (predominantly existing data and new data being generated by the EPA HPV, OECD SIDS, and ICCA HPV programs). The products in this category are very similar to the products in the American Petroleum Institute Petroleum HPV Testing Group Gasoline Testing Plan. A significant amount of data already exists for the streams included in the gasoline test plan. These data are expected to be sufficient to characterize the human health hazards of the products included in this category in satisfaction of the HPV program requirements.

No additional human health studies are proposed to characterize the streams in this category.

Physiochemical Properties, Environmental Fate, and Aquatic Toxicity

Existing measured data will be identified to adequately characterize physicochemical endpoints in the HPV Program. In addition, calculated data will be developed to characterize the physiochemical endpoints for selected chemicals in products from this category and compared with existing measured data.

The strategy for characterizing the biodegradability and aquatic toxicity of products in this category is to evaluate data on component chemicals contained by products in this category and similar complex products.

Read across biodegradation data show that products in the Low Benzene Naphtha Category have the potential to exhibit a high extent of biodegradability.

Read across aquatic toxicity data show that products in the Low Benzene Naphtha Category have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute

toxicity in freshwater fish and invertebrates.
The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment.

Information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to characterize these endpoints consistent with the Panel's voluntary HPV commitment.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the test plan for the "Low Benzene Naphtha" Category under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category.

This category test plan addresses nine petrochemical streams (products) derived from the ethylene and associated manufacturing processes. The category includes products that are complex chemical mixtures containing primarily C5 through C12 olefinic, paraffinic, naphthenic and aromatic molecules. The aromatic components account for the major chemical class ranging from approximately 45 percent to 95 percent. The benzene content is usually less than five percent.

It will be possible to characterize the HPV Chemical Program endpoints for all products in this category using existing information plus data that will be developed as outlined in this test plan.

Human Health Effects

The strategy of this test plan for characterizing the human health hazards of the products in this category is to evaluate data from similar products and/or several of the components of products in this category (existing data and new data that will be generated as part of the EPA HPV, OECD SIDS, and ICCA HPV programs). These data are expected to be sufficient to characterize the human health hazards of the substances included in this category in satisfaction of the HPV program requirements.

Based upon examinations of stream compositions and existing toxicity data for similar materials as well as some of the components of streams in the Low Benzene Naphtha Category, there is minimal likelihood for the appearance of unexpected or remarkable biological findings in testing of streams within this chemical class.

No additional human health studies are proposed to characterize the streams in this category.

Physiochemcial Properties, Environmental Fate, and Aquatic Toxicity

Existing measured data will be identified to adequately characterize physicochemical endpoints in the HPV Chemical Program. In addition, calculated data will be developed to characterize the physiochemical endpoints for selected chemicals in products from this category and compared with the existing measured data.

The strategy for characterizing the biodegradability and toxicity of products in this category is to

evaluate data on component chemicals contained by products in this category and similar complex products.

Read across biodegradation data show that products in the Low Benzene Naphtha Category have the potential to exhibit a high extent of biodegradability.

Read across aquatic toxicity data show that products in the Low Benzene Naphtha Category have the potential to produce a moderate level of toxicity in freshwater algae and a moderate level of acute toxicity in freshwater fish and invertebrates.

The chemical components in these products are relatively volatile, and if released they would be expected to partition to the air phase to a significant extent. In the air, they are subject to rapid physical degradation through hydroxyl radical attack. Therefore, as a result of both biological and physical degradation processes, these products are not expected to persist in the environment.

Information has not been developed on the potential of products in this category to photodegrade, hydrolyze, and partition within the environment. Therefore, information or data will be developed to characterize these endpoints consistent with the requirements of the HPV program.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

ATOFINA Petrochemicals, Inc.*
BP Chemical Company
Chevron Phillips Chemical Company LP
The Dow Chemical Company
E. I. du Pont de Nemours and Company*
Eastman Chemical Company*
Equistar Chemicals, LP
ExxonMobil Chemical Company
Formosa Plastics Corporation, U.S.A.
The Goodyear Tire & Rubber Company*
Huntsman Corporation
Koch Industries
NOVA Chemicals Inc.*
Noveon, Inc.*
Sasol North America, Inc.*
Shell Chemical Company
Sunoco, Inc.*
Texas Petrochemicals Corporation*
Westlake Chemical Corporation*
Williams Olefins, LLC*

* These companies are part of the Olefins Panel but do not produce streams in the Low Benzene Naphtha Category.

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I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the Low Benzene Naphtha Category under the Environmental Protection Agency (EPA) High Production Volume (HPV) Challenge Program (Program).

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than a rote checklist approach. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for substances included in the category, and outlines testing needed to develop screening level data for this category under the Program. This document also provides the testing rationale for the Low Benzene Naphtha Category. The objective of this effort is to identify and develop sufficient test data and/or other information to characterize the human and environmental health and environmental fate for the category in accordance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in EPA guidance documents. In addition, measured data will be provided for selected products in this category when available.

II. DESCRIPTION FOR THE LOW BENZENE NAPHTHA CATEGORY

A. The Category

The Low Benzene Naphtha Category was developed for the HPV program by grouping ethylene manufacturing streams that exhibit commonalities from both manufacturing process and compositional perspectives. The ten CAS numbers listed in Table 1 each represent at least one production stream. All of these process streams are complex products containing many chemical components. CAS numbers are used to represent these stream products, but are assigned vague verbal descriptions for distinguishing the streams. Certain single streams may be correctly represented by more than one CAS number, and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix I.

The streams in this category consist of complex hydrocarbon reaction products that are predominantly

C5 through C12. Aromatics represent the major constituents in all of the streams, varying from approximately 45 to 95 percent. The benzene content is usually less than five percent. The typical compositions of the streams are shown in Table 2. The category is designated Low Benzene Naphtha.

The CAS Numbers in the Low Benzene Naphtha Category are associated with nine streams that are commercial products or isolated intermediates:

1. Pyrolysis C7s
2. Pyrolysis C7-C12
3. Pyrolysis C7-C8
4. C9+ From Xylene Unit
5. Hydrotreated C8-C10
6. Hydrotreated C7-C12
7. Hydrotreated C7+
8. Hydrotreated C5/C9 blend
9. Toluene Extract

Descriptions of the nine streams associated with the Low Benzene Naphtha category are presented below:

(1)-(3) Pyrolysis C7s, C7-C12, and C7-C8 Fractions: Pyrolysis gasoline is separated by distillation into various boiling-point-range fractions as an intermediate step in preparation for further processing. Many carbon number distribution fractions are technically feasible. The compositions of these fractions vary depending on the ethylene process feedstock, the cracking furnaces operating conditions and the ethylene process configuration.

(1) Pyrolysis C7s: The reported composition is 75% toluene with the balance primarily C7 non-aromatics, largely unsaturates. The stream may contain low levels of benzene.

(2) Pyrolysis C7-C12 Fraction: The typical composition reported included about 2% benzene, 23% toluene, 28% C8 aromatics and 8% naphthalene. The balance expected to be largely unsaturated hydrocarbons and other aromatics.

(3) Pyrolysis C7-C8 Fraction: The reported compositions indicate C7-C8 streams that contain 45 to 80% toluene and other streams with 11 to 78% C8 aromatics. The typical benzene concentration reported was 2% with a maximum of 5%.

(4) C9+ from Xylene Unit: This stream is a coproduct from process units that produce o- or p-xylene. The carbon distribution for the stream is C8 to hydrocarbon compounds with a boiling point of 65F or higher. The stream is predominantly aromatics.

(5)-(8) Hydrotreated Pyrolysis Fractions (Hydrotreated C8-C10, C7-C12, and C7+Fractions, and C5/C9 Blend): Pyrolysis gasoline, or distillate fractions of pyrolysis gasoline are typically treated with hydrogen over catalyst. The hydrogenation process may be either a one-stage or two-stage. The one-stage process is typically a liquid-phase process where the primary objective is to selectively convert diolefins to mono-olefins and to convert, for example, styrene to ethylbenzene. The two-stage process is typically a vapor-phase, more severe hydrogenation that hydrogenates essentially all of the contained mono- and diolefins to paraffins. A pygas fraction that will be processed by extraction or extractive distillation to produce aromatics (toluene or xylenes in this case) is subject to two-stage hydrogenation. Pygas fractions may be forwarded to hydrodealkylation units (less common) for benzene production after one-stage of hydrogenation. Pygas fractions intended for use as a gasoline blending stock are frequently subject to only one-stage hydrogenation. The streams may result from fractionation of hydrotreated pyrolysis gasoline or from hydrotreating pyrolysis gasoline fractions followed by distillation. Reformate fractions from Petroleum refineries are sometimes mixed with these pyrolysis fractions.

(5) Hydotreated C8-C10 Fraction: The carbon number distribution for this stream C6 -C12, but is predominately C8-C10. The reported typical concentration includes 0.3% benzene, 2.4% toluene, 24% C8 aromatics with the balance primarily and C9 and C10 aromatics and lesser amounts of paraffins, isoparaffins and naphthenes in this carbon range.

(6) Hydrotreated C7-C12 Fraction: The carbon number distribution for this distillate fraction of hydrogenated pygas is predominately C7- C12, with lesser amounts of C6. The reported typical concentration includes 1% benzene, 23% toluene, 25% C8 aromatics, with the balance primarily other aromatics and lesser amounts of monoolefins and paraffins.

(7) Hydrotreated C7+ Fraction: This stream is derived as distillation residue after removing the C5 and C6 fractions from a hydrogenated pygas stream. (Alternately the stream could be hydrotreated after distillation.) The carbon number distribution is predominantly greater than C6, although the reported analysis does not report compounds greater than C12. The reported typical analysis includes 23% toluene, 32% C8 aromatics, 1% naphthalene, with the balance primarily other aromatics and lesser amounts of paraffins.

(8) Hydrotreated C5/C9 Blend: This stream is produced by blending C5 and C9 pyrolysis fractions, hydrogenated either before or after blending. Reported typical analysis includes about 2% benzene, 40% C5's in the blend, 9% C8 aromatics, 19% C9 aromatics, and 25% C10+.

(9) Toluene Extract: This stream is produced as a co-product of a benzene extraction unit. The stream may contain significant concentrations of xylenes.

III. TEST PLAN RATIONALE

A. Human Health Effects - Overview

A substantial amount of toxicity data are available for many of the components of the streams in the Low Benzene Naphtha Category. Some of the components are SIDS materials, and some components will be tested by other category test plans or by other groups within the EPA or ICCA HPV programs. In addition, a significant amount of testing has already been completed on hydrocarbon streams of similar composition and boiling point ranges.

The American Petroleum Institute (API) Petroleum HPV Testing Group is sponsoring a group of materials under the Gasoline Blending Streams Test Plan that are very similar to the materials included in the Low Benzene Naphtha Category. Not surprisingly, some of the streams in the Low Benzene Naphtha Category are used as gasoline blending stock. The substances included in the Gasoline Blending Streams test plan are all volatile hydrocarbon liquids at standard temperature and pressure and are referred to as naphthas. These streams have a boiling range of -20 ºC to 230 ºC and a carbon number distribution of predominantly C4-C12. These blending streams are all complex mixtures and contain many different components. The API Petroleum HPV Testing Group has categorized these materials into four groups; **p**araffinic, **o**lefinic, **n**aphthenic and **a**romatic. These chemical classes are often abbreviated and referred to collectively by the acronym PONA. Product streams are placed into one of the above categories based on the predominant chemical composition type. It is important to note that naphthas enriched in one chemical class also contain components of other classes.

Adequate data already exist for the naphtha streams enriched in either paraffins, olefins or aromatics and additional testing is being proposed by the API Petroleum HPV Testing Group for streams with relatively high content of naphthenes (cycloparaffins). The streams in the Low Benzene Naphtha Category are most similar in composition to the high aromatic class of streams referenced in the Gasoline Blending Streams test plan, though they still maintain some similarities with the other blending streams. The API Petroleum Test Group has identified several streams in the high aromatic group for which data exist, including Full Range Catalytic Reformed Naphtha (FRCRN), Light Catalytic Reformed Naphtha (LCRN), and Heavy Catalytic Reformed Naphtha (HCRN). The FRCRN typically consists of approximately 63 percent aromatic, with approximately 2 percent benzene. The remaining material consists of approximately 32 percent paraffins, 0.5 percent olefins and 4 percent naphthenes. The carbon number range is predominantly C5 through C12. The LCRN and HCRN contain approximately 31 and 93 percent aromatic content, respectively. The streams in the Low Benzene Naphtha Category contain 45 –95 percent aromatics, 5-20 percent paraffins, <1 –38 percent olefins and <1-45 naphthenes, a carbon number range of C5 through C12 and a typical benzene content of 2%.

Results of studies on naphtha streams high in aromatic constituents are briefly summarized below (For additional details and robust summaries see the Gasoline Blending Streams Test Plan submitted by The American Petroleum Institute Petroleum HPV Testing Group).

1. Acute Toxicity

The high aromatic stream, also referred to as full range catalytic reformed naphtha (FRCRN) is relatively non-toxic after acute oral (rat = 3500-9800 mg/kg), dermal (rabbit > 2000 mg/kg) and inhalation (rat > 5.22 mg/L 4-hour exposures) exposure routes. These materials are non-irritating to eyes and moderate skin irritants. They are not skin sensitizers in guinea pigs.

2. Genetic Toxicity – Gene Mutation

Light catalytic reformed naphtha (42% aromatic) did not induce mutatgenic events in the mouse lymphoma (L5178Y TK+/-) forward mutation assay with or with out metabolic activation. Full range catalytic reformed naphtha (63% aromatic) was negative in the absence of metabolic activation and positive in the presence of metabolic activation. Heavy catalytic reformed naphtha (90% aromatics) gave positive and equivocal results with and without activation, respectively.

3. Genetic Toxicity – Chromosome Aberration

Full range, catalytic reformed naphtha, light catalytic reformed naphtha and heavy reformed naphtha were tested in rat chromosome aberrations assays via intraperitoneal injection. None of these materials induced chromosome aberrations.

4. Repeated Dose Toxicity

Full range catalytic reformed naphtha was evaluated in a 28-day dermal toxicity study (New Zealand White rabbit) at doses of 0, 200, 1000, and 2000 mg/kg/day, 3 days/week. Moderate to severe skin irritation was noted. Three males (2 high dose, 1 mid dose) died. Histopathologic examination revealed slight-moderate proliferative and inflammatory changes in skin at the highest dose concurrent with granulopoiesis of bone marrow, attributed to stress and other factors associated with skin irritation. No other significant findings were noted.

FRCRN was also evaluated in a 13-week inhalation study using Sprague-Dawley rats. Animals were exposed to the volatile fraction (partially vaporized to simulate human exposure) at concentrations of 0, 96, 464 and 1894 ppm (0, 410, 1970, and 8050 mg/m^3) 5 days/week. Higher kidney and liver weights were noted in the high dose males. However, no treatment related abnormalities were observed in any tissue upon histological examination.

Sprague-Dawley rats were exposed by inhalation for 21 days (15 exposures) to light catalytic reformed naphtha (31% aromatics) and heavy catalytic reformed naphtha (93% aromatics) at concentrations of 0, 544, 1591, and 5522 ppm (0, 2000, 5850, and 20300 mg/m^3) and 0, 215, 587, and 2132 ppm (0, 1030, 2810, and 10200 mg/m^3), respectively. LCRN induced small concentration-related increases in necrosis of renal tubules and an increased incidence and severity of hyaline droplets, typical of light hydrocarbon nephropathy. No adverse kidney effects were noted after exposure to HCRN however, lung irritation was apparent. In a 13-week study, Sprague-Dawley rats were exposed to a light vapor

fraction of LCRN at concentrations of 0, 750, 2500, and 7500 ppm (0, 2775, 9250 and 27,750 mg/m^3). No test article related mortality or effects on physical signs, body weight, food consumption or clinical chemistry were observed. A significant decrease in white blood cell and lymphocyte counts and a decrease in spleen weight were observed at terminal sacrifice in males exposed to 7500 ppm, but were not present in animals after a 4-week recovery period. Statistically significant increases in kidney weight relative to body weight in high dose males correlated with microscopically observed light hydrocarbon nephropathy. The only effect on neurobehavioral parameters was significantly higher motor activity in the high dose males after the four-week recover period. However, there was no evidence of hyperactivity or abnormal behavior from the functional observation battery and no microscopic changes in neural tissue.

Results of repeat-dose dermal studies of gasoline blending streams with relatively high aromatic content indicate that these materials are generally skin irritants with systemic effects primarily related to skin damage and accompanying stress. Inhalation studies of gasoline blending streams with predominant aromatic content show minimal toxicity with the exception of light hydrocarbon nephropathy in male rats. This effect is believed to be a species and sex specific effect and is not relevant to human health. No neurobehavioral or neuropathological effects were observed. Repeat-dose studies performed on gasoline blending streams with high olefinic or high paraffinic content (results non summarized) had findings similar to the high aromatic content streams.

5. Reproductive and Developmental Toxicity

FRCRN was tested in a developmental toxicity screen by exposing pregnant Sprague-Dawley rats to partially vaporized FRCRN via inhalation at concentrations of 0, 508 and 1835 ppm (0, 2160, 7800 mg/m^3) on gestation days 6-19. Animals were sacrificed on day 20 of gestation. Maternal body weights, serum chemistry, and organ weights were unaffected. No adverse effects were observed on fetal parameters at sacrifice (viability, fetal body weight, external development) or subsequent skeletal and visceral examinations.

A distillate of light catalytic reformed naphtha administered to male and female Sprague-Dawley rats by inhalation at target concentration of 0, 750, 2500, and 7500 ppm (0, 2775, 9250 and 27,750 mg/m3) according to OECD protocol 421, did not affect reproductive performance, delivery data or live pups/litter. Offspring showed comparable body weights, weight gain, and viability at postnatal day four. Parental systemic effects observed at the highest dose were slightly reduced body weights for males, increased kidney to body weight and liver to body weight ratios. No histological changes were seen in reproductive organs of treated rats.

Reproductive and developmental toxicity studies with gasoline blending streams high in olefinic or parafinic content (data not summarized) had similar findings.

Existing data are expected to be sufficient to characterize the human health hazards of the substances included in this category for purposes of satisfying HPV requirements.

B. Physical-Chemical Properties

The physicochemical (PC) endpoints in the HPV Chemical Program include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Water Solubility
- Octanol/Water Partition Coefficient (K_{ow})

Although some of these data exist for products in the Low Benzene Naphtha Category, not all of these endpoints are defined, and a comprehensive and consensus database for chemicals that represent product streams in this category does not exist. Therefore, calculated PC data for selected component chemicals in this category will be developed using a computer model to provide a consistent, representative data set. In addition, measured PC data will be identified for selected products in this category and will be summarized together with the calculated data to provide comparisons between the two data sets. The selection of component chemicals to be modeled will be made once an appropriate measured data set is identified.

Calculated PC data for selected component chemicals in the Low Benzene Naphtha Category will be developed using EPIWIN© computer model,[1] as discussed in the US EPA document entitled "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program."[2] The use of computer modeling for the development of these data is justified since components of the streams in this category are all chemically related and are expected to exhibit relatively similar environmental properties. In addition, a calculated dataset provides a common method in the development of these values for all the chemicals selected to represent products in this category.

Boiling point, melting point, and vapor pressure ranges will be determined using the MPBPVP subroutine in EPIWIN. K_{ow} and water solubility will be calculated using KOWIN and WSKOW subroutines, respectively. There is more information on calculating data for the HPV chemical program in the EPA document titled, "The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program."

Because the HPV substances covered under the Low Benzene Naphtha Category testing plan are mixtures containing differing compositions, it is not possible to develop or calculate a single numerical value for each of the physicochemical properties. For example, a product that is a mixture of chemicals does not have a melting point, but rather a melting range. Calculated values for physicochemical properties will be represented as a range of values according to the product's component composition and based on the results of computer modeling. Robust summaries characterizing the PC endpoints will be prepared upon completion of a review of available measured data, and will include the calculated and measured data.

C. Environmental Fate

The environmental fate endpoints in the HPV Chemical Program include:

- Biodegradation
- Photodegradation
- Hydrolysis
- Fugacity

Although biodegradation data are not available for products in the Low Benzene Naphtha Category, there are data for selected component chemicals of those products, as well as for complex products, that can be used to characterize the potential biodegradability of products in this category. The complex product values are for substances composed of a range of chemicals with regard to carbon number and chemical classes (i.e., paraffins, alkenes, and alkylbenzenes). As suggested by the experimental data, products in this category will exhibit a significant extent of biodegradation.

Data or information for the fate endpoints, photodegradation and hydrolysis will have to be developed and will be either calculated and/or discussed in technical summaries. Chemicals in this category are not subject to hydrolysis at measurable rates, therefore, information for this endpoint will be summarized in a technical review document.

Equilibrium models are used to calculate chemical fugacity, which can provide information on where a chemical is likely to partition in the environment. These data are useful in identifying environmental compartments that could potentially receive a released chemical. Fugacity data can only be calculated for individual chemicals. For the HPV Chemical Program, environmental partitioning data will be developed for selected component chemicals of the products in this category.

A preliminary evaluation of chemicals in the Low Benzene Naphtha Category suggests that they will partition largely to the air, and therefore their fate in air is of environmental interest. Because the air phase may be a compartment that could potentially receive many of the component chemicals in this category, data characterizing their potential for physical degradation in the atmosphere will be developed (this is discussed below under photodegradation).

1. Biodegradation

There are sufficient data to characterize the potential biodegradability of products in this category. Data for constituent chemicals of products in this category, as well as for complex products not in this category that contain chemicals found in products from this category, suggest that low benzene naphtha products have the potential to biodegrade to a great extent (Table 3). The carbon number of products in this category ranges primarily between C5 to C11. Results for several chemicals with carbon numbers in this range that are contained by these products have been shown to biodegrade from 63 to 100% after

14 or 28 days, while results for several complex products range from 21 to 96% after 28 days. As seen by the data in Table 3, there is a relatively large biodegradation dataset for single chemicals and complex products that can be used to characterize this endpoint for the low benzene naphtha products. These data best describe the potential biodegradability of the low benzene naphtha products, because products in this category are compositionally more comparable to the products identified in Table 4 as gasoline streams. Gasoline compositions are provided in Table 2.

The data from the majority of tests in Table 3 were developed using a manometric respirometry test procedure. This procedure uses continuously stirred, closed systems, which is recommended when assessing the potential biodegradability of chemically complex, poorly water soluble, and volatile materials like those in this category. Stirring is recommended when evaluating products containing several chemicals, some of which may have limited water solubility.

2. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline.[3]

To develop information or data that will characterize the potential of products in this category to undergo direct photochemical degradation, the existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The UV light absorption of selected chemicals in products in the Low Benzene Naphtha Category will be evaluated to identify those chemicals with a potential to degrade in solution. When possible, first order reaction rates will be calculated for chemicals identified to have a potential for direct photolysis in water. The results of the calculation will be summarized in a technical discussion for this endpoint. If instead, a low potential for direct photolysis is suggested by the evaluation, a technical discussion will be prepared to summarize the findings.

3. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured[4] (the US EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the US EPA.[2] An estimation method accepted by the US EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Hydrocarbons, such as those in the Low Benzene Naphtha Category, have the potential to volatilize to air where the can react with hydroxyl radicals (OH-).

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows)[1] is used by

the US EPA OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for representative chemical components of products in the Low Benzene Naphtha Category. The existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The resulting calculations will be summarized in a robust summary for this endpoint.

4. Hydrolysis

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters.[5] Chemical stability in water can be measured (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA.[4] An estimation method accepted by the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows)[1] is used for this purpose by OPPTS.

All of the chemical structures included in the Low Benzene Naphtha Category are hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

5. Chemical Transport and Distribution in the Environment - Fugacity Modeling

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The US EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model.[6] The U.S. EPA cites the use of this model in its document titled Determining the Adequacy of Existing Data,[4] which was prepared as guidance for the HPV Chemical Program.

In its document, U.S. EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments described above within a defined unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties

including molecular weight, melting point, vapor pressure, and water solubility to calculate distribution within a unit world. This model will be used to calculate distribution values for representative chemical components identified in products from this category. Existing product chemical composition data will be evaluated to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. A computer model, EPIWIN version 3.04,[1] will be used to calculate the physicochemical properties needed to run the Level I EQC model.

6. Aquatic Toxicity

The aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

Although aquatic toxicity data are not available for products in the Low Benzene Naphtha Category, there are sufficient read across data from both constituent chemicals of those products and comparably complex products to fully characterize the toxicity of this category. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class or combinations of chemical classes (i.e., olefins, aromatics, paraffins) that are found in products from this category.
- Individual chemicals and complex products used for read across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in products from this category.
- Individual chemicals and complex products used for read across purposes as well as the products in this category are composed chemicals that all act by a similar mode of toxic action.

The data in Table 5 provides a comparison of the range of product compositions (i.e., carbon number, chemical class, weight percent) in the Low Benzene Naphtha Category to products that will be used to characterize the aquatic toxicity of this category. This comparison illustrates the similarity in carbon number ranges between products in this category and the selected products

with read across data. The data in Tables 6, 7 and 8 establish the range of toxicity that products in this category will demonstrate, based on the read across data.

The aquatic toxicity data presented in this test plan fall within a narrow range of values regardless of their varying chemical class content and carbon number range. This is not unexpected, because the constituent chemicals of products in this category are neutral organic hydrocarbons whose toxic mode

of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function,[7] and the differences

between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals.[8]

The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight, [9,10] supporting the assessment that these chemicals have equal potencies. When normalized to lipid content, the CBR is approximately 50 umol of hydrocarbon/g of lipid for most organisms.[11] Because the products in this category are all complex mixtures containing relatively similar series of homologous chemicals, their short-term toxicities are expected to fall within the range of toxicity demonstrated by the individual chemicals, as well as comparable products summarized in this test plan. Therefore, the existing data are believed to form a sufficiently robust dataset to fully characterize the aquatic toxicity endpoints in the HPV Chemical Program for this category.

The fish and invertebrate acute and alga toxicity values for individual chemicals and complex products similar to those in this category (Tables 6, 7, 8) fall within a range of approximately 1-46 mg/L and overlap between the three trophic levels. Because the products in the Low Benzene Naphtha Category will range in paraffin, alkene, and/or aromatic carbon number content within approximately C5 to C12, a range in toxicity for products in this category will be comparable to the range of data summarized in Tables 6, 7 and 8.

As suggested by the experimental data, this category will exhibit a moderate range of acute toxicity to fish and invertebrates and a moderate range of toxicity to algae. For representative chemicals and products, experimental acute fish toxicity values range between 2.5 to 46.0 mg/L for two species (Table 6), while acute invertebrate toxicity values range between 0.9 to 32 mg/L for one species (Table 7). In comparison, alga toxicity values for one species range between 1.0 to 64 mg/L (for biomass or growth rate endpoints), while alga NOELR values range between 1.0 to 51 mg/L (for biomass and growth rate endpoints) (Table 8).

Generally, the fish, invertebrate, and alga studies followed the OECD Guidelines 203, 202, and 201, respectively. For complex products, the test procedures used to develop the test material exposure solutions also applied the OECD guidance described in "Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures."[12] For these studies, the results are represented as lethal loading (LL) endpoints, compared to the data developed for pure
chemicals, that represent results as lethal concentration endpoints where test material is analytically verified.

IV. TEST PLAN SUMMARY

The following evaluations, testing, modeling, and technical discussions will be developed for the Low Benzene Naphtha Category (Table 9):

- Evaluate data for the SIDS human health endpoints obtained for similar products and or components and prepare a technical discussion in terms of their representation of potential human health effects for streams in this category.

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program*. Identify available measured physicochemical data for representative products of this category. Identify readily available measured physiochemical data for products in this category.

- Prepare a technical discussion on the potential of component chemicals comprising streams in this category to photodegrade.

- Prepare a technical discussion on the potential of component chemicals comprising streams in this category to hydrolyze.

- Calculate fugacity data for selected component chemicals of streams in this category.

This test plan identifies data to characterize the human health effects and environmental effects and biodegradation endpoints for the Low Benzene Category under the HPV program. Data for selected physicochemical and environmental fate endpoints will be identified and/or developed. After these data have been developed, all data associated with this category will be evaluated to determine whether they support the category for the HPV Chemical Program endpoints or if additional data or testing is needed.

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Table 1.
CAS Numbers and Descriptions Associated with Streams in the Low Benzene Naphtha Category

CAS Number	CAS Number Description
64741-98-6	Extract, petroleum, heavy naphtha solvent
64742-48-9	Naphtha, petroleum, hydrotreated heavy
64742-49-0	Naphtha, petroleum, hydrotreated light
64742-83-2	Naphtha, petroleum, light steam-cracked
68333-88-0	Aromatic hydrocarbons, C9-C17
68476-45-9	Hydrocarbons, C5-10 aromatic concentrate, ethylene manufacture by-product
68478-10-4	Naphtha, petroleum, light steam-cracked, debenzenized, C8-16-cycloalkadiene concentrate
68516-20-1	Naphtha, petroleum, steam-cracked middle aromatic
68527-23-1	Naphtha, petroleum, light steam cracked aromatic
68919-15-3	Hydrocarbons, C6-12, benzene-recovery

Note: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition)

Table 2. Typical Stream Compositions (wt. %) for the Low Benzene Naphtha Category.

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
C4's								0.2 - 3.6	
C4 and C5		2							
Isopentane (2-methylbutane)								3 - 7	
1-Pentene (Amylene)								0.5 - 1	
2-Methyl-1-Butene								1 - 2	
Pentene-2 (isomer mix)								7 - 15	
Pentane								2 - 5	
2-Methyl-2-Butene								4 - 8	
Cyclopentene								4 - 8	
Cyclopentane								1 - 3	
2-methylpentane								0.5 - 4	
3-methylpentane (Isohexane)								0.1 - 1	
C6 Hydrocarbons		9							
Hexane		4			3.7				
Remaining C6 to C7 non-Aromatic Hydrocarbons			0.2 - 12						
Benzene		1.5 - 2	5		0 - 0.4	1		3	<0.1
Cyclohexane					1				
heptenes						5			
2-methylhexane						5			
Heptane						2	1 - 3		
C8								3	
C7 Olefins	25								
i-octane						5			

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
C7-Non-aromatics		1							
Toluene	75	22 - 23	45 - 80		2.4	20 - 25	15 - 30		75-80
nonaromatics			10 - 20						
C8 Paraffins & Naphthenes		35			0.1				
C8 olefin					0.8				
Octane							1		
Ethylbenzene		3 - 5	7 - 25		2.4 - 10.7	10 - 15	10 - 20	9	5-20
C8 Aromatics				0.9					
C9 Olefins					3.3				
i-nonene						5			
Xylenes, mixed		9 - 17	3.5 - 45		3.3 - 17.9	10 - 15	10 - 20	0.3 - 3	5-20
C8's		1							
Styrene		10 - 11	0.5				1 - 3	0.5 - 5	
isopropylbenzene (cumene)					0.9		1 - 3		
C10 Isoparaffins					1.1				
Propylbenzene				1.8	3 - 3.5		1 - 3		
C9 Aromatics					4.6	10 - 20		19	
Ethyltoluenes				52.82	6		1 - 5		
C9 Paraffins and Naphthenes					2.3				
1,4-methylethylbenzene					9.4				
C10+		17						25	
C-10 Naphthenes					4.9				
1,2,4-Trimethylbenzene (pseudocumene)		3							
Trimethylbenzenes				4.4	5		2 -4		
Dicyclopentadiene							1 - 3	1 - 4	
Vinyl Toluene							1		

Component Name	Pyrolysis C7s	Pyrolysis C7-C12	Pyrolysis C7-C8 Fraction	C9+ from O-xylene Unit	Hydro-treated C8-C10	Hydro-treated C7-C12	Hydro-treated C7+	Hydro-treated C5/C9 Blend	Toluene Extract
Propenylbenzene							2		
C9's		10							
Indane (indan)					8.5				
sec-butylcyclohexane					8.8				
3-ethylnonane					1.5				
C9+ Parafins				2.88					
C9+ Naphthenes				0.94					
C9+ Aromatics				96.18					
C10 Aromatics					1.8	10 - 20			
C-11 Isoparaffins					18				
diethylbenzenes					1.3				
Indene							2		
dimethyl-ethylbenzenes					0.8				
C10-C11 Alkylbenzenes							13 - 35		
C11+ Aromatics						10 - 15			
Naphthalene		7 - 9		11.5	0.2 - 7.8		2	0.2 - 4	
tricyclodecane					44				
2-Methylnaphthalene				8.7					
1,1'-Biphenyl				0.5					
C10 Parafins & Naphthenes					0.8				
Heavy Hydrocarbons and Polycyclic Aromatics				22.4					

Note 1:The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 2: The listed ranges should not be considered absolute values. They are instead the approximate highs and lows of the reported values, and are expected to be typical limit values.
Note 3: The definitions, found in the TSCA Chemical Substance Inventory, for the CAS numbers included in this group are vague with respect to composition. Therefore, it is not uncommon to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the stream

(composition).

Table 3.
Read Across Data used to Characterize the Biodegradability of the Low Benzene Naphtha Category
from Chemicals Contained by Products in this Category and Chemically Complex Products not in this Category, but that Contain Like-Chemicals.

CHEMICAL / PRODUCT	CARBON NUMBER	PERCENT BIODEGRADATION(a) (28 days)	REFERENCE
n-Pentane	5	87	IHSC*
Isopentane	5	71	IHSC*
Cyclohexane	6	77	IHSC*
Alkenes, C6 Rich	6(b)	21	HOP**
1-Hexene (linear)	6	67-98(c)	12****
Benzene	6	63	*****
Alkenes, C7-C9, C8 Rich	7-9	29	HOP**
p-Xylene	8	89	IHSC*
Styrene	8	100 (14 days)(c)	12****
Naphtha (Petroleum), light alkylate (gasoline stream)	5-8	42(d)	API***
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8	74(d)	API***
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-9	96(d)	API***
C8-C10 Aromatics, Predominantly C9 Alkylbenzenes	9(b)	78	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(b)	61	IHSC*

a OECD 301F, manometric respirometry test
b Predominant carbon number or range
c BOD test
d Test method for determining the inherent aerobic biodegradability of oil products and modification of ISO/DIS 14593
* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)
** Robust summary from the Higher Olefins Panel: C6, C7, C8, C9, and C12 Internal Olefins and C16 and C18 Alpha Olefins Category Test Plan (submitted)
*** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)
**** These chemicals are in the OECD SIDS program
***** Robust summary submitted with Olefins Panel's High Benzene Naphtha Category Test Plan

Table 4.
Composition (Weight Percent) of Three Gasoline Streams with Biodegradation Data Used to Read Across to Products in the Low Benzene Naphtha Category.

Naphtha, (Pet.) Light Alkylate		Naphtha, (Pet.) Light Catalytically Cracked		Naphtha, (Pet.) Light Catalytically Reformed	
CAS# 64741-66-8	Weight %	CAS# 64741-55-5	Weight %	CAS# 64741-63-5	Weight %
Isopentane	12.61	n-hexane	1.69	n-heptane	3.59
2,3 dimethyl butane	4.74	n-pentane	1.71	n-hexane	4.69
2,4 dimethyl pentane	4.09	isopentane	4.7	n-pentane	8.05
2,3 dimethyl pentane	2.25	2,3 dimethyl pentane	1.12	Isopentane	11.39
2,2,4 trimethyl pentane	23.92	2 methyl hexane	1.58	2,2 dimethyl butane	1.26
2,2,3 trimethyl pentane	1.76	3 methyl hexane	1.45	2,3 dimethyl butane	1.11
2,3,3 trimethyl pentane	8.99	2 methyl pentane	3.64	2,3 dimethyl pentane	1.70
2,3,4 trimethyl pentane	11.56	3 methyl pentane	2.20	2 methyl hexane	4.30
2,3,5 trimethyl hexane	1.25	methyl cyclopentane	1.87	3 methyl hexane	5.18
2,5 dimethyl hexane	4.34	methyl cyclohexane	1.19	2 methyl pentane	5.17
2,4 dimethyl hexane	3.60	1-pentene	1.25	3 methyl pentane	4.00
2,3 dimethyl hexane	2.60	2-methyl-1-butene	2.31	benzene	8.37
1methyl-1ethyl cyclopentane	9.44	2-methyl-2-butene	5.35	toluene	29.77
		trans-2-pentene	3.33		
		cis -2-pentene	1.94		
		2-methyl-1-pentene	2.31		
		cis -3-hexene	1.67		
		trans-2-hexene	1.97		
		2-methyl-2-pentene	1.83		
		1-methyl cyclopentene	1.85		
		ethylbenzene	1.47		
		m-xylene	3.05		
		p-xylene	1.34		
		o-xylene	1.83		
		benzene	1.48		
		toluene	6.73		

Table 5.
Approximate Weight Percent and Carbon Number Comparison of Hydrocarbons in Low Benzene Naphtha Category and Comparable Products (a).

Substance Name	Olefins		Aromatics		Paraffins	
	% (wt.)	C # (b)	% (wt.)	C # (b)	% (wt.)	C # (b)
Products in Low Benzene Naphtha Category	1-34	5-9	>40-100	6-11	>4-75	5-10
Alkenes, C6 Rich	100	5-7	0	-	0	-
Alkenes, C7-9, C8 Rich	100	7-9	0	-	0	-
C8-C10 Aromatics, Predominantly C9 Aromatics	0	-	>97	8-10	<3	-
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	0	-	>94	10-14	<6	-
Naphtha (petroleum), Light Alkylate (gasoline stream)	0	-	0	-	92	5-8
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	24	5-6	16	6-8	21	5-7
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	0	-	38	6-7	50	5-7

a Approximate weight percent and carbon number ranges of the predominant chemical components by chemical class [olefins/aromatics/paraffins] for selected products contained by this category and for comparable products not in this category that have aquatic data that can be used as read across data for this category; % compositions may not total 100%.
b Predominant carbon number range

Table 6.
Acute Fish Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the Low Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (96-hr, mg/L)	REFERENCE
n-Pentane	5	*Oncorhynchus mykiss*	LC50 = 4.3	IHSC*
n-Hexane	6	*Pimephales promelas*	LC50 = 2.5	IHSC*
Benzene	6	*Oncorhynchus mykiss*	LC50 = 5.9	13****
Alkenes, C6 Rich	5-7(b)	*Oncorhynchus mykiss*	LL50 = 12.8	HOP**
Mixed Cycloparaffins, C7-8, C7 Rich	7	*Oncorhynchus mykiss*	LC50 = 5.4(c)	IHSC*
Toluene	7	*Pimephales promelas*	LC50 = 14.6	IHSC*
Alkenes, C7-9, C8 Rich	7-9(b)	*Oncorhynchus mykiss*	LL50 = 8.9	HOP**
o-Xylene	8	*Pimephales promelas*	LC50 = 16.4	IHSC*
p-Xylene	8	*Oncorhynchus mykiss*	LC50 = 2.6	IHSC*
p-Xylene	8	*Pimephales promelas*	LC50 = 8.9	IHSC*
Ethylbenzene	8	*Pimephales promelas*	LC50 = 12.1	IHSC*
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(b)	*Pimephales promelas*	LL50 = 8.2	API***
Naphtha (petroleum), Light Catalytically Cracked (gasoline stream)	5-8(b)	*Pimephales promelas*	LL50 = 46	API***
Naphtha (petroleum), Light Catalytically Reformed (gasoline stream)	5-7(b)	*Pimephales promelas*	LL50 = 34	API***
1,2,4-Trimethyl-benzene	9	*Pimephales promelas*	LC50 = 7.7	IHSC*
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(b)	*Oncorhynchus mykiss*	LL50 = 18.0	IHSC*
C8-C14 Aromatics,	10-12(b)	*Oncorhynchus*	LL50 = 3.0	IHSC*

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (96-hr, mg/L)	REFERENCE
Predominantly alkyl Naphthalenes and Naphthalene		*mykiss*		

a Endpoint is mortality; LC = Lethal Concentration; LL = Lethal Loading; NOELR = No Observed Effect Loading Rate; values cited as "concentration" are based on measured values
b Predominant carbon number or range
c 93-hour value
* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)
** Robust summary from the Higher Olefins Panel HPV Test Plan (submitted)
*** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)
**** Benzene is in the OECD SIDS program

Table 7.
Acute Invertebrate Toxicity Data for Selected Chemicals and Complex Products used to Characterize the Toxicity of Products in the Low Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (48-hr, mg/L)	REFERENCE
n-Pentane	5	*Daphnia magna*	EC50 = 2.7	IHSC*
n-Hexane	6	*Daphnia magna*	EC50 = 2.1	IHSC*
Cyclohexane	6	*Daphnia magna*	EC50 = 0.9	IHSC*
Benzene	6	*Daphnia magna*	EC50 = 18(b)	13***
o-Xylene	8	*Daphnia magna*	EC50 = 1.0	IHSC*
m-Xylene	8	*Daphnia magna*	EC50 = 4.7	IHSC*
Naphtha (Petroleum), Light Catalytically Reformed (gasoline stream)	5-7(c)	*Daphnia magna*	EL50 = 10	API**
Naphtha (Petroleum), Light Alkylate (gasoline stream)	5-8(c)	*Daphnia magna*	EL50 = 32	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	*Daphnia magna*	EL50 = 18	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	*Daphnia magna*	EL50 = 21.3	IHSC*
Naphthalene	10	*Daphnia magna*	EL50 = 16.7(d)	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	*Daphnia magna*	EL50 = 3.0	IHSC*

a Endpoint is immobility; EC = Effect Concentration; EL = Effect Loading; NOELR = No Observed Effect Loading Rate; values cited as "concentration" are based on measured values
b 24-hour study
c Predominant carbon number or range
d Based on nominal values
* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)
** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)
*** Benzene is in the OECD SIDS program

Table 8.
Alga Toxicity Data for Selected Chemicals and Complex Products Used to Characterize the Toxicity of Products in the Low Benzene Naphtha Category.

CHEMICAL / PRODUCT	CARBON NUMBER	ORGANISM	AQUATIC TOXICITY (a) (72-hr, mg/L)	REFERENCE
n-Pentane	5	*Pseudokirchneriella subcapitata(b)*	EbC50 = 10.7 ErC50 = 7.5 NOECb = 1.3 NOECr = 2.0	IHSC*
Benzene	6	*Pseudokirchneriella subcapitata*	EbL50 = 29	13***
Naphtha (Petroleum), Light Catalytically reformed (gasoline stream)	5-7(c)	*Pseudokirchneriella subcapitata*	EbL50 = 8.5 NOELRb = 5.0	API**
Naphtha (Petroleum), Light alkylate (gasoline stream)	5-8(c)	*Pseudokirchneriella subcapitata*	EbL50 = 45 NOELRb = 18	API**
Naphtha (Petroleum), Light Catalytically Cracked (gasoline stream)	5-8(c)	*Pseudokirchneriella subcapitata*	EbL50 = 64 NOELRb = 51	API**
C8-C10 Aromatics, Predominantly C9 Aromatics	8-10(c)	*Pseudokirchneriella subcapitata*	EbL50 = 2.6 ErL50 = 2.9 NOELRb = 1.0 NOELRr = 1.0	IHSC*
C8-C14 Aromatics, Predominantly Alkyl Naphthalenes and Naphthalene	10-12(c)	*Pseudokirchneriella subcapitata*	EbL50 = 1-3 ErL50 = 1-3 NOELRb = 1.0 NOELRr = 1.0	IHSC*

a Endpoint is growth inhibition; EbC = Effect Concentration for biomass); ErC = Effect Concentration for growth rate; EbL = Effect Loading for biomass; ErL = Effect Loading for growth rate; NOEC(b) = No Observed Effect Concentration for biomass; NOEC(r) = No Observed Effect Concentration for growth rate; NOELR(b) = No Observed Effect Loading Rate for biomass; NOELR(r) = No Observed Effect Loading Rate for growth rate; values cited as "concentration" are based on measured values

b Formally known as *Selenastrum capricornutum*

c Predominant carbon number or range

* Robust summary from the International Hydrocarbon Solvents Consortium: Contained in selected SIAR (to be submitted)

** Robust summary from the American Petroleum Institute: Gasoline Test Plan (to be submitted)

*** Benzene is in the OECD SIDS program

Table 9. Assessment Plan for Low Benzene Naphtha Category Under the Program. Robust summaries for existing studies are submitted separately.

Stream Description	Human Health Effects						Ecotoxicity			Environmental Fate				
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.[1]	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Pyrolysis C7s	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C7-C12	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Pyrolysis C7-C8	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
C9+	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C8-C10	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C7-C12	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C7+	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Hydrotreated C5/C9 blend	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA
Toluene Extract	RA	RA	RA	RA	RA	RA	RA	RA	RA	CM	CM/TD	TD	CM	RA

1 Measured data for selected physicochemical endpoints will be identified in conjunction with calculated data.

Ö Adequate existing data available TD Technical Discussion proposed RA Read Across

CM Computer modeling proposed

Table 10. Existing Human Health Effects Data for Gasoline Blending Streams.
(Robust summaries for these studies will not be submitted with the Test Plan but will be submitted by the American Petroleum Institute (API) Petroleum HPV Testing Group in support of the Gasoline Blending Streams test plan.)

	Human Health Effects					
Chemical Name	Acute Oral	In vitro mouse lymphoma	In vivo - Genetic Chrom. Aberr.	Sub chronic	Developmental	Reproduction
Naphtha light alkylate (high paraffinic)	√	√	√	√	√	√
Naphtha light catalytic cracked (high olefinic)	√	√	√	√	√	√
Naphtha heavy straight- run (high naphthenic)						
Full range catalytic reformed naphtha (high aromatic)	√	√	√	√	√	
Light catalytic reformed naphtha (high aromatic)		√	√	√	√	√
Heavy catalytic reformed naphtha (high aromatic)		√	√	√		

Table 11. American Chemistry Council Olefins Panel Sponsored HPV Test Categories.

Category Number	Category Description
1	Crude Butadiene C4
2	Low Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (C3) - Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, & 9	Resin Oil & Cyclodiene Dimer Concentrates
10	Fuel Oils

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturates. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers".

Subjecting the feedstocks to high temperatures results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the liquid feedstocks are also converted to ethylene. While the predominant products produced are ethylene and propylene, a wide range of additional products are also formed. These products range from methane (C1) through fuel oil (C12 and higher) and include other olefins, diolefins, aromatics and saturates (naphthenes and paraffins).

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins from refinery gas streams, such as from the light ends product of a catalytic cracking process or from coker offgas. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked

gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges and in some cases further processed. It is a subset of these mixed streams that make up the constituents of the Low Benzene Naphtha Category.

The chemical process operations that are associated with the process streams in the Low Benzene Naphtha Category are shown in Figure 1.

Figure 1. Chemical Process Operations Associated with Process Streams in the Low Benzene Naphtha Category.